Interim Practical Quantitation Level (PQL) determination to support Interim Specific Ground Water Quality Standard development for Perfluorooctane Sulfonate (PFOS)

New Jersey Department of Environmental Protection
Division of Science and Research

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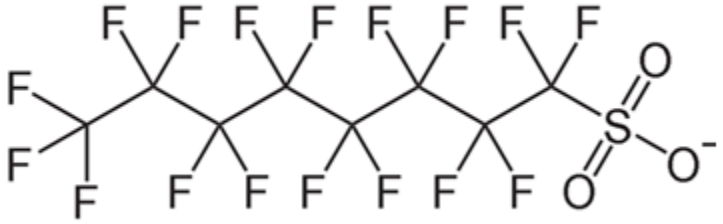

The New Jersey Department of Environmental Protection (Department) develops an interim Practical Quantitation Level (PQL) and Interim Specific Ground Water Quality Criterion when the need for an Interim Ground Water Quality Standard is identified (i.e., for a contaminant that is not included in the Ground Water Quality Standards [GWQS]: N.J.A.C. 7:9 Appendix Table 1). As per the GWQS, all standards and PQLs are rounded to one significant digit.

Derivation of PQL: The method detection limit (MDL) and the PQL are performance measures used to estimate the limits of performance of analytical chemistry methods for measuring contaminants. The MDL is defined as "the minimum concentration of a substance that can be measured and reported with 99 percent confidence that the analyte concentration is greater than zero" (40 CFR Part 136 Appendix B). For PQL development, USEPA recommends that an MDL be multiplied by a factor of five or ten to account for the analytical variability and uncertainty that can occur when attaining a quantifiable concentration.

A laboratory performance data solicitation is initiated for compounds of interest to collect sufficient data to calculate a PQL. The Department utilizes these data as an indication of the quantification capabilities of the laboratory community by comparison to literature reviews that reflect the latest advances in analytical capability for the parameter of interest. The requested laboratory performance data includes MDL, low point on the calibration curve, and more recently reporting limits (RL). Both, the low point on the calibration curve and the RL are quantifiable concentrations. An RL can theoretically be equivalent to the lowest point on the calibration curve, but RL values are often higher. This is because RL are often client driven and requested for specific data evaluation needs, which may not be as sensitive as the low point on the calibration curve. Therefore, RL may not meet the data quality objectives of the Department, especially when these values are higher than the human health criteria developed through the Department risk assessment process.

The performance data is often highly skewed with many low values and only a few relatively higher values. Skewed data will bias an average value and thus the mean will not accurately

reflect the central tendency of the measure. A median, or 50th percentile, of the data is free of bias and a preferable measure of central tendency when data is highly skewed. In order to achieve a level of confidence around the central value, one can utilize bootstrapping, or iterative random sampling with replacement, to estimate the mean of the interlaboratory data to generate a normal distribution, free of the skewed bias, so that a representative mean and upper 95% confidence level (UCL) can be estimated. Bootstrapping is a useful analytical approach that allows for familiar statistical calculations based upon the normal distribution produced by the method.

NJDEP has typically multiplied the median of the interlaboratory MDL acquired from the New Jersey certified laboratory community by a factor of five to derive an individual PQL. Utilizing bootstrapping methods allows for other PQL derivations as listed in the table below. A bootstrap estimate of the UCL of the average interlaboratory MDL can be multiplied by five to provide a reliable quantitation level that most laboratories can be expected to meet with 95% certainty. A bootstrap UCL of the average low point on the calibration curves as well as the simple median and mean of the low point on the calibration curve are also presented as PQL estimates. No multiplicative factor is included in PQL derivations on the low point of a calibration point because it represents a quantifiable value. The UCL of the average RL is also presented as a PQL estimate. No multiplicative factor is included in PQL derivations on RL because it represents a quantifiable value

PQL Derivation Approach	**Number of Laboratories**	**Value (ng/L)**
Median MDL (1.0 ng/L) x 5	13	5
Bootstrap Upper Confidence Limit of MDL (0.76 ng/L) x 5	7	4
Median of the reported lowest calibration standard	15	4
Mean of the reported lowest calibration standard	13	4
Bootstrap Upper Confidence Limit of Low Point Calibration Curve	11	4
Bootstrap Upper Confidence Limit of Reporting Limit	8	4
Median of the six (6) Quantification Methods		4

The PQLs based on the low point of the calibration curve and generated from the bootstrap UCL are then compared to the method based on the median MDL (multiplied by 5) that has been used by the Department in the past. Of note, the bootstrap technique used to determine the concentration level encompassing the certified laboratory community's quantification capability with greater than 95% confidence (UCL) is 4 ng/L and is consistent with and complements the Department's approach of PQL calculation using N.J.A.C. 7:9C-1.9(c)3ii (2).

Sufficient interlaboratory performance data was collected from thirteen (13) laboratories to **recommend an interim PQL of 4 ng/L for perfluorooctane sulfonate (PFOS)** in groundwater using modified USEPA method 537 and Department Sanctioned Analytical Methods (DSAMs). PFOS also appears as a listed parameter in proprietary method standard operating procedures from three laboratories.

Note: Analytical results reported for perfluorooctanesulfonic acid (the acid form) are applicable to perfluorooctane sulfonate (the anion form).